Ising Model

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Abstract. A serial and parallelizable algorithms for the Ising model are presented. The differences in these algorithms are compared while varying several simulation parameters.

1 Introduction

The Ising model is a describes heat-induced phase transitions ferromagnetic materials. The model assumes that atoms in a lattice each contribute one electron which may either be spin up or spin down. While nonlocal interactions may be modeled as well, the most simplistic model considers only nearest-neighbor interactions. For the 1D case, it has been shown that phase transitions do not occur; however, for two and three dimensions, phase transitions have been shown to occur []. In general, the analytical solutions to this model are difficult and require functional analysis, however Monte-Carlo techniques exist that enable the determination system properties numerically [].

1.1 Ising Model

For the spin configuration $\sigma = \{\sigma_1, \sigma_2, \cdots\}$ where the σ_j are the atomic spin states, the generic Hamiltonian of the system is given by

$$H(\sigma) = -\sum_i \sum_j J_{ij}\sigma_i\sigma_j - \mu \sum_i h_i\sigma_i \tag{1}$$

where J_{ij} is a matrix which determines the intensity of interactions and geometry of the system, h_i is the intensity of an external magnetic field and μ is an scalar[]. The partition function is then given by

$$Q(N,T) = \sum_{\sigma\in\Sigma} \mathrm{e}^{-\beta H(\sigma)} \tag{2}$$

where Σ is the set of all valid $\underbrace{N \times N \times \cdots \times N}_{d}$ configurations in d dimensions. Means that there are N^d binary values to consider meaning that $\mathrm{card}(\sigma) = 2^{N^d}$ which is *very* large even for small systems. The probability of each states is then given by

$$P(\sigma) = \frac{\mathrm{e}^{-\beta H(\sigma)}}{\sum_\sigma \mathrm{e}^{-\beta H(\sigma)}}, \tag{3}$$

and we define the magnetization of a state to be

$$M(\sigma) = \Big| \sum_j \sigma_j \Big|. \tag{4}$$

Shown in [] there is a critical temperature.

1.2 Metropolis Algorithm

Due to the intractability of the set Σ, induces a requirement to find a way of sampling Σ which finds configurations with high probabilities. The metropolis algorithm does just that. The Metropolis algorithm begins with an initial spin configuration, and, then, a new configuration is proposed. If the energy of the new configuration is lower, the configuration is accepted, otherwise it may be accepted or rejected randomly. Through this process, a new set Σ^* is created which, in practice, has similar statistics to that of Σ while being much, much smaller.

Formally, for a set X, the Metropolis algorithm generates a Markov chain which contains elements of X. Let g be the proposal distribution, that is, we propose a new member of $x' \in X$ using the distribution $g(x'|x)$. For the existence of a stationary distribution, it is sufficient to require $g(x|y) = g(y|x)$[], that is, the probability of proposing y given that the current state is x is equal to the probability of proposing x given that the current state is y. Let f be a function proportional to the probability density, then the Metropolis algorithm is given as follows:

1. Given $x^n \in X$ generate a new proposal $x' \in X$.
2. Calculate the acceptance ratio $\alpha = \frac{f(x')}{f(x^n)}$.
3. If the random number $r \in [0, 1]$ is such that $r \leq \alpha$, let $x^{n+1} = x'$ otherwise, let $x^{n+1} = x^n$.

Starting from $x^0 \in X$, it is easy to see how we can generate a sequence $X^* = \{x^0, x^1, \dots\}$ where for all $x \in X^*$ we have $x \in X$ []. Heuristically, if $x \in X$ is highly probable, it will appear be represented many times in X^*, and conversely, if x is not probable, it will be represented few times in X^*.

2 Methods

2.1 Modeling and Simulation

Consider an $N \times N$ system of spins states each of which may be spin-up or spin-down which we represent by 1 and -1, respectively. Let σ be some configuration of the Ising model is initialized with totally random spins and wrapped with periodical boundary. With $J_{i,j} = 1$ for nearest neighbors and zero everywhere else, and $\mu_j = \mu$ for all j, the energy of the configuration σ is given by

$$H(\sigma) = \sum_{\langle ij \rangle} J\sigma_i\sigma_j + \sum_j \mu h \sigma_j. \tag{2.1.1}$$

The term $\sum_i \sigma_i$ can be determined by counting total possible configuration states for each three by three micro-canonical ensemble, see fig 1.

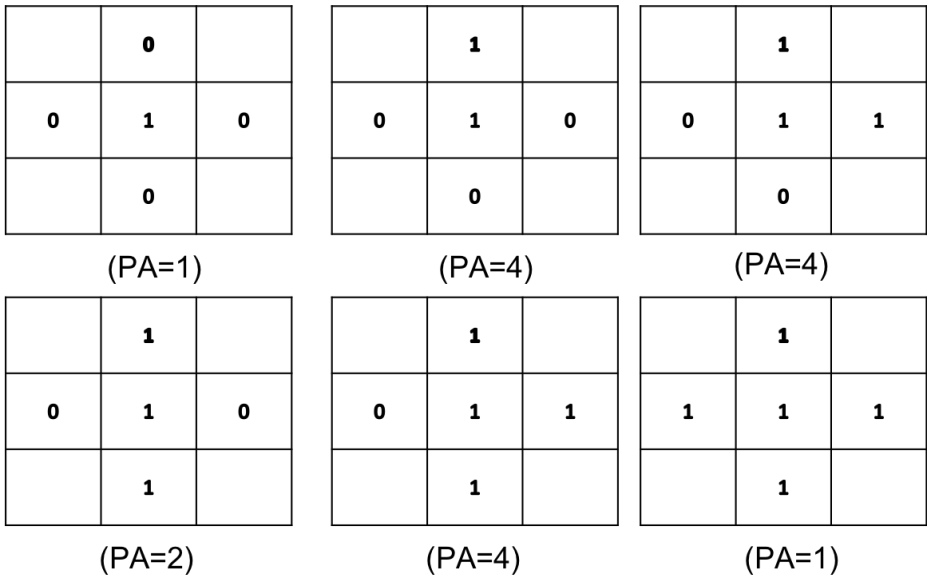

Fig. 1. Possible configuration states for micro-canonical ensemble. There are total six possible configuration for energy calculation. Number 1 represents this neighbor is aligned with σ_j, number 0 represents this neighbor is not aligned with σ_j. PA represents the possible alignment for this configuration.

From the six possible configuration states, the Hamiltonian is obtained by summing up the spins of all four first neighbors, see fig 2. For each configuration, the partition function of micro canonical ensemble can be calculated using equation 2.1.2. By calculating the energy change by flipping σ_j then we can assign Monte-Carlo moves to the system, and the probability is given in equation 2.1.3:

$$\Lambda = e^{-\beta H} = e^{-\beta(\sum_{ij} J\sigma_i\sigma_j + \sum_j \mu h\sigma_j)} \tag{2.1.2}$$

Where $\beta = \frac{1}{k_B T}$, where k_B is Boltzmann's constant and T is absolute temperature.

$$P(\sigma_j) = \frac{1}{2}\frac{\Lambda(\sigma_j)}{\Lambda(-\sigma_j)} \tag{2.1.3}$$

We randomly choose a number from zero to one to compare to $P(\sigma_j)$. If the number is smaller than $P(\sigma_j)$, then we accept the flip of the spin,otherwise, we reject the flip. In order to smooth the data, 10 different simulations with the same initial state but different initial configuration are accumulated and averaged. Different step size, temperature, and μ are assigned to carry out a

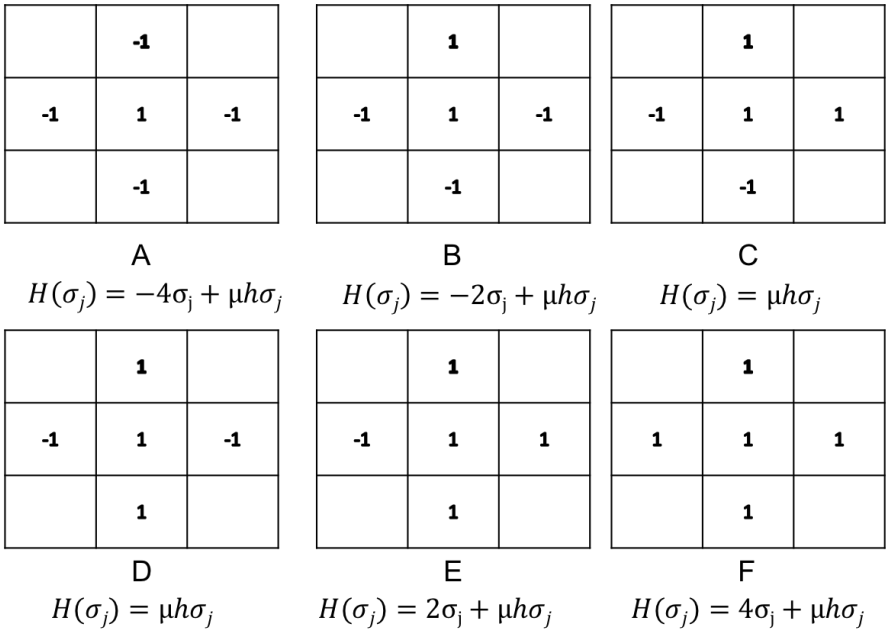

Fig. 2. Spins for each possible configuration. Considering the symmetry, a "mirror" state must be count for each configuration by flipping all five atoms at the same time, this gives the exact same configuration with the exact same energy. In this case, we can just divide by 2 for each configuration to get rid of the over-counting states.

comparative study. For another approach, the partition function of canonical ensemble is evaluated and further the probability for all possible configurations is calculated using equation 2.1.4 and 2.1.5:

$$q(\sigma_j) = \sum_{\sigma_j} e^{-\beta H(\sigma_j)} \tag{2.1.4}$$

$$P = \frac{\Lambda}{q(\sigma_j)} = \frac{e^{-\beta H}}{\sum_{\sigma_j} e^{-\beta H(\sigma_j)}} \tag{2.1.5}$$

2.2 Method B

The second method, while more robust is not feasible for large systems.

Let A be the set (ensemble) of all $N \times N$ matrices filled with elements from the set $\{-1, 1\}$. To do this we constructed all binary sequences of length N^2 which we parsed into an array of length N^2, and, then, reshaped into an $N \times N$ array. We then calculated the probabilities using the partition function. Due to overflow error it is not feasible to use the partition function directly. Instead, recall the state probabilities is related to the partition function. Let $\sigma \in A$, then

$$P(\sigma) = \frac{\mathrm{e}^{-\beta H(\sigma)}}{\sum_\sigma \mathrm{e}^{-\beta H(\sigma)}} \tag{2.1.6}$$

Let σ^* be the value of such that $H(\sigma^*)$ is minimized. It is not necessary that σ^* is unique. However, it is necessary that H exists. In this case, we are guaranteed existence since there are only finitely many different sequences of length N^2. Then

$$\begin{aligned}
\ln(P(\sigma)) &= \ln\left(\frac{\mathrm{e}^{-\beta H(\sigma)}}{\sum_\sigma \mathrm{e}^{-\beta H(\sigma)}}\right), \\
&= -\beta H(\sigma) - \ln\left(\sum_\sigma \mathrm{e}^{-\beta H(\sigma)}\right), \\
&= -\beta H(\sigma) - \ln\left(\mathrm{e}^{-\beta H(\sigma^*)} \sum_\sigma \mathrm{e}^{-\beta(H(\sigma)-H(\sigma^*))}\right), \\
&= -\beta(H(\sigma) - H(\sigma^*)) - \ln\left[\sum_\sigma \mathrm{e}^{-\beta(H(\sigma)-H(\sigma^*))}\right]. \qquad (2.1.7) \\
& \qquad (2.1.8)
\end{aligned}$$

Since $H(\sigma^*)$ is the minimum value of H, it must be the case that $H(\sigma) - H(\sigma^*) \geq 0$ which implies $\mathrm{e}^{-\beta(H(\sigma)-H(\sigma^*))} \leq 1$; consequently, $\sum_\sigma \mathrm{e}^{-\beta(H(\sigma)-H(\sigma^*))} \leq N^2$. If we then calculate the probabilities using the following formula, overflow errors are much less of an issue:

$$P(\sigma) = \exp\left\{-\beta(H(\sigma) - H(\sigma^*)) - \ln\left[\sum_\sigma \mathrm{e}^{-\beta(H(\sigma)-H(\sigma^*))}\right]\right\}. \tag{2.1.9}$$

3 Results

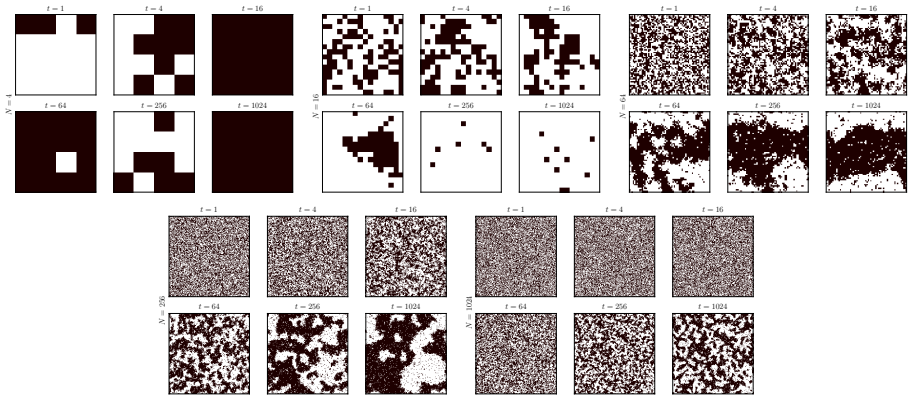

Fig. 3. $\beta = 0.5$,$\mu = 0$

4 Analysis

4.1 Method Comparison

5 Conclusion

References

1. Example, F., Ekeland, I.: Nonlinear oscillations and boundary-value problems for Hamiltonian systems. Arch. Rat. Mech. Anal. 78, 315–333 (1982)